Supplementary Information

Mechanochromism in the luminescence of novel cyclometalated platinum(II) complexes with α-aminocarboxylates

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2. Figures

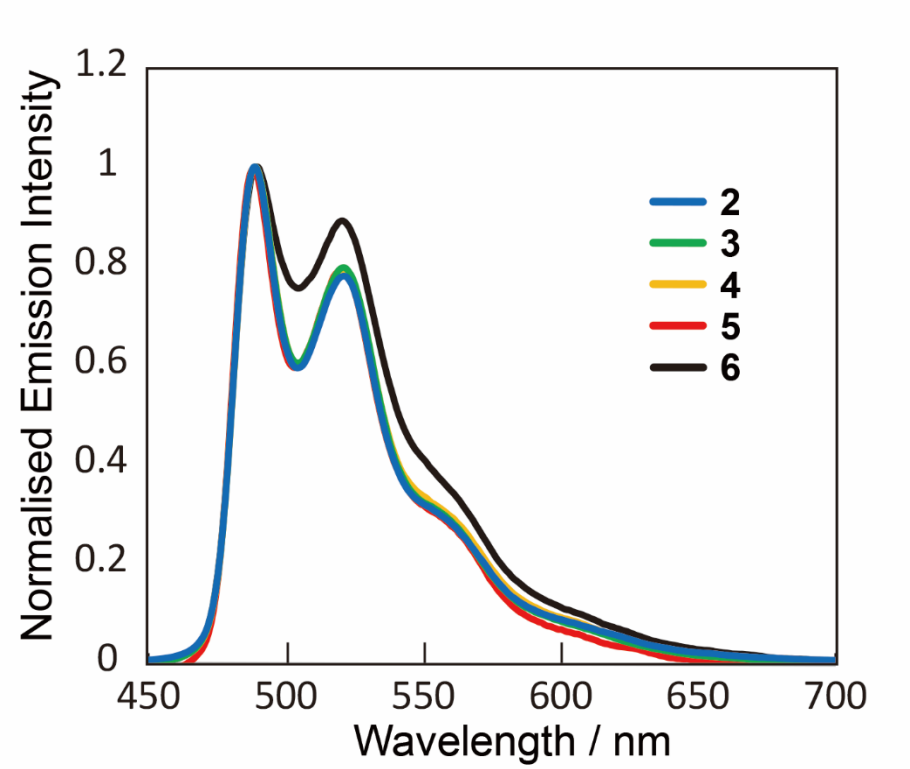

Fig. S1 Emission spectra (λ_{ex} = 400 nm) in MeOH/EtOH mixed solution (v/v = 1:1, 1.0 × 10^{-5} M) at room temperature of **2** (blue), **3** (green), **4** (yellow), **5** (red), and **6** (black).

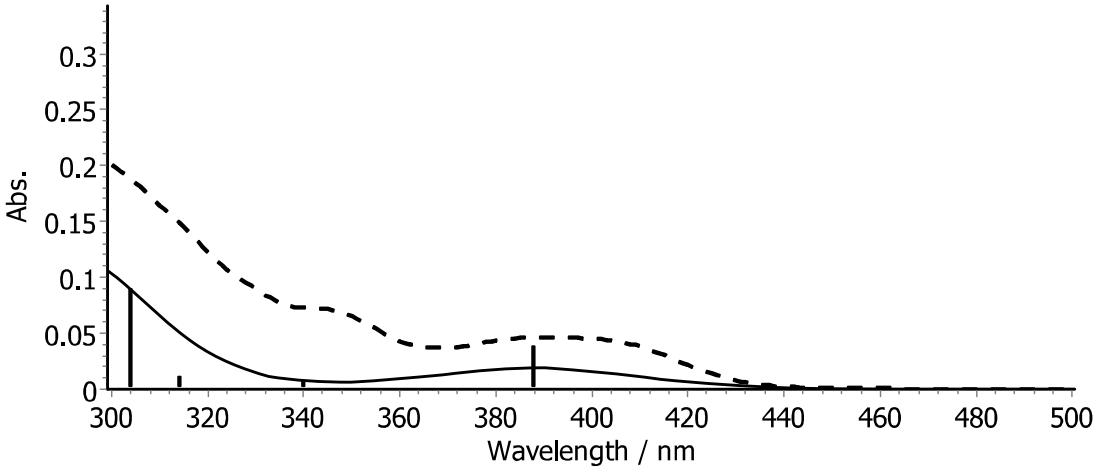

Fig. S2 Calculated UV-vis absorption spectrum (line) with TD-DFT calculation and experimental UV-vis absorption spectrum (dashed black) of **1** in DMSO

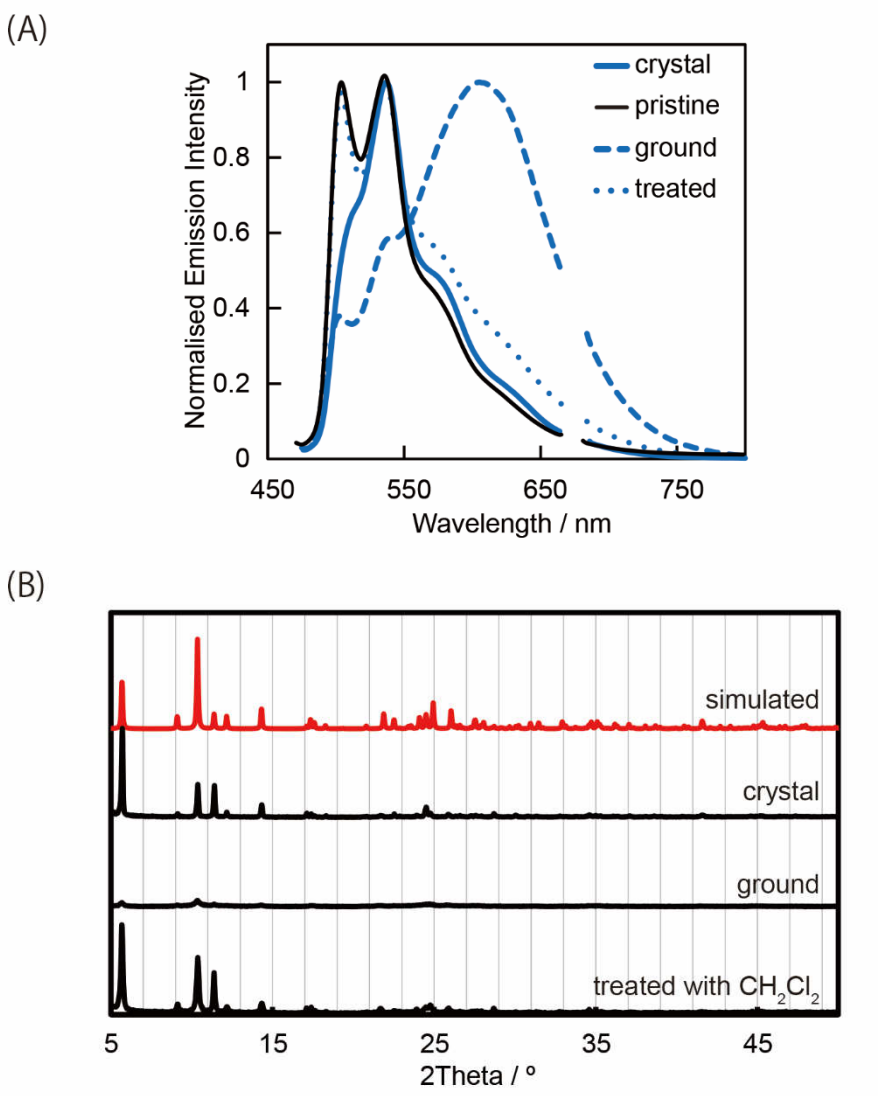

Fig. S3 (A) Luminescence spectral changes of **2** upon mechanical grinding and treatment with CH_2Cl_2 (λ_{ex} = 365 nm). (B) Changes in XRD patterns by mechanical grinding and solvent treatment for **2**.

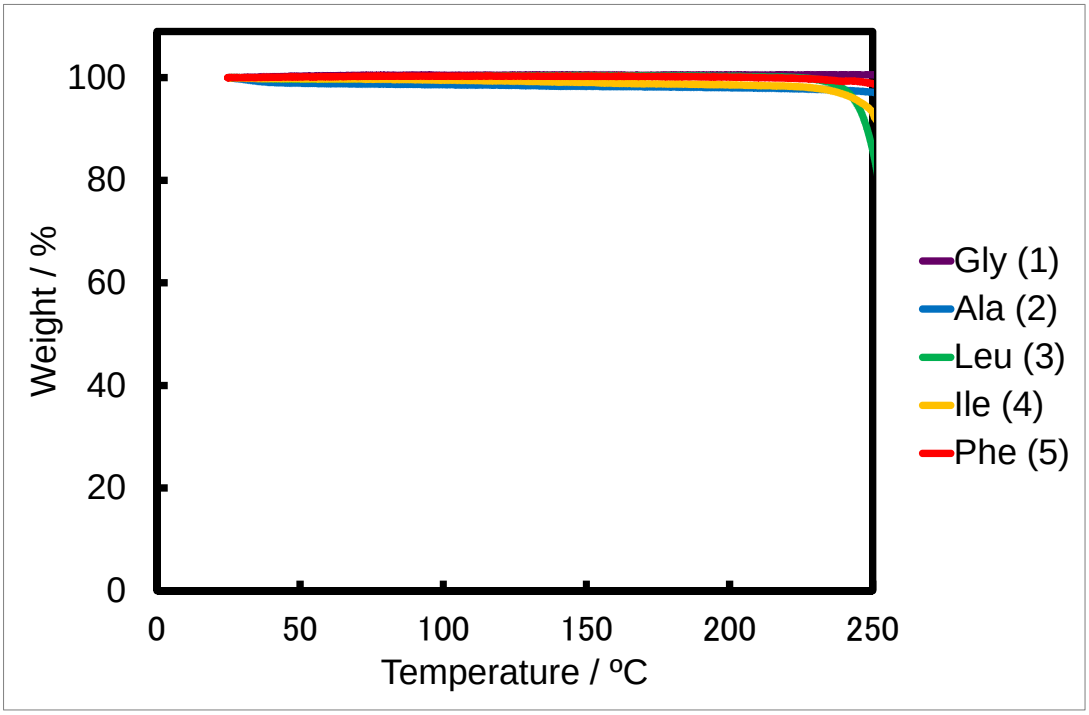

Fig. S4 Thermogravimetric analyses for **1**–**5** in crystalline state.

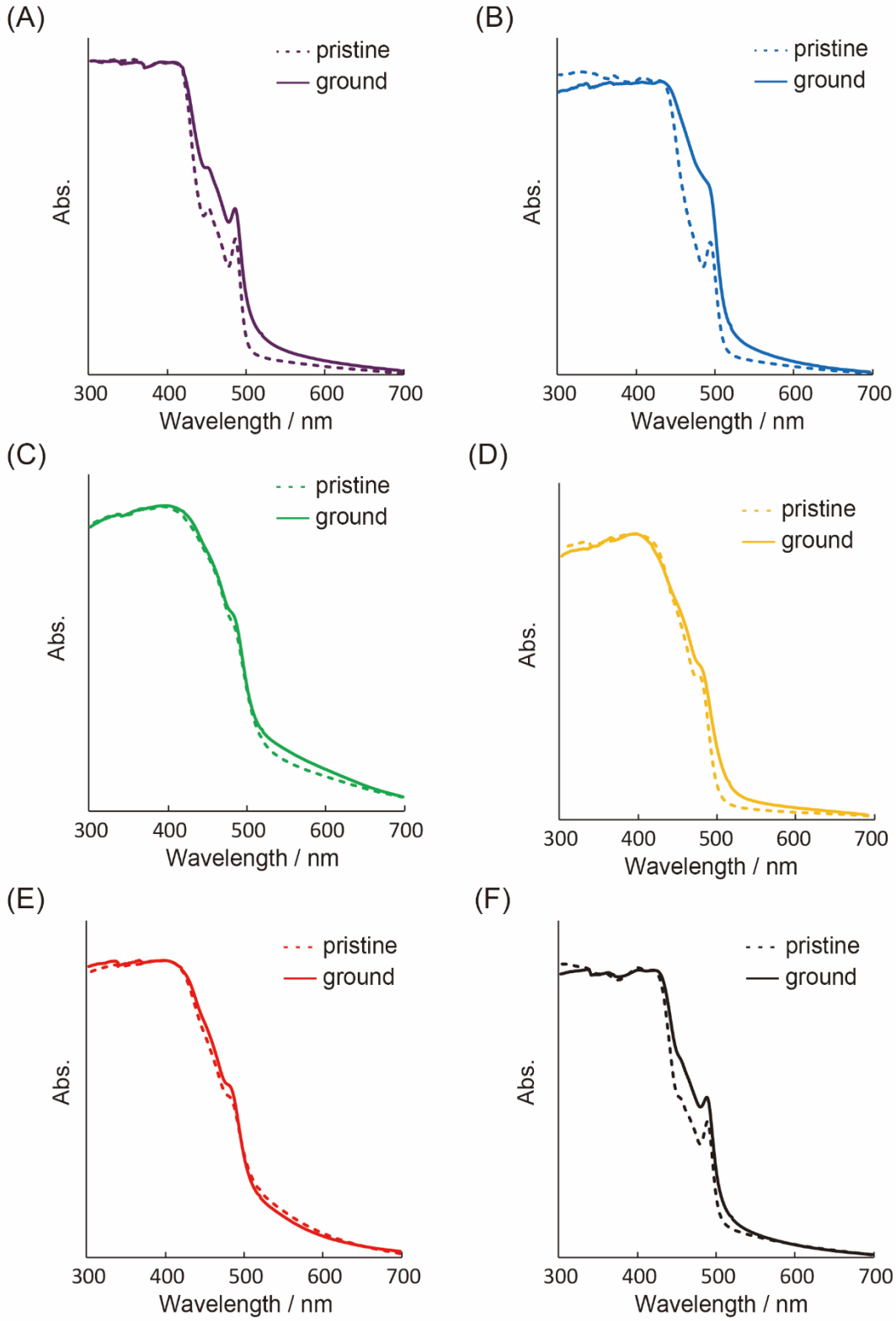

Fig. S5 UV-vis absorption spectral changes of the pristine samples **1** (A), **2** (B), **3** (C), **4** (D), **5** (E), **6** (F) by grinding.

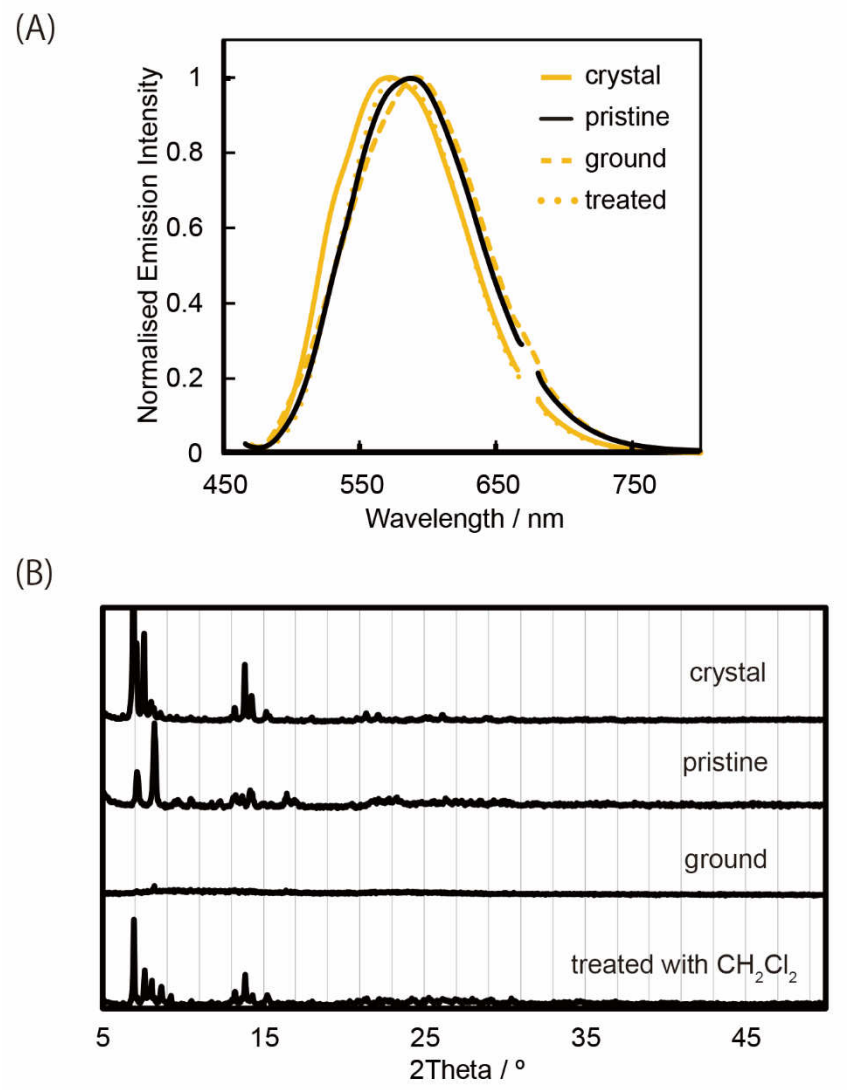

Fig. S6 (A) Luminescence spectral changes of **4** upon mechanical grinding and treatment with CH_2Cl_2 (λ_{ex} = 450 nm). (B) Changes in XRD patterns by mechanical grinding and solvent treatment for **4**.

3. Tables

Table S1 Partial molecular orbital compositions (%) in the ground state of **1** in DMSO.

		Contribution (%)		
Orbital	Energy (eV)	Pt	ppy	glycinato
LUMO+5	0.60	51	39	7
LUMO+4	0.42	53	11	27
LUMO+3	−0.07	25	63	9
LUMO+2	−0.12	40	32	22
LUMO+1	−1.08	2	98	0
LUMO	−1.77	6	93	1
HOMO	−5.74	50	40	10
HOMO−1	−6.32	95	2	3
HOMO−2	−6.49	25	70	5
HOMO−3	−6.64	15	4	79
HOMO−4	−6.78	72	24	2
HOMO−5	−7.08	45	17	37

Table S2 Summary of crystallographic data for **1**, **2**, **3**, and Crystals-G and -Y.

	1	**2**	**3**
formula	$C_{13}H_{12}N_2O_2Pt$	$C_{14}H_{14}N_2O_2Pt$	$C_{17}H_{20}N_2O_2Pt$
formula weight	423.34	437.36	479.44
temperature (K)	200	200	200
crystal system	Monoclinic	Orthorhombic	Tetragonal
space group	*Cc*	*P*2(1)2(1)2(1)	*P*4(3)
a / Å	36.350(3)	4.0937(4)	18.330(4)
b / Å	4.1921(4)	10.2147(9)	18.330(4)
c / Å	17.1948(16)	31.067(3)	20.570(5)
α / º	90.00	90.00	90.00
β / º	116.6000(10)	90.00	90.00
γ / º	90.00	90.00	90.00
V / Å^3	2342.9(4)	1299.1(2)	6912(3)
Flack parameter	0.5	0.014(10)	0.004(17)
Z	8	4	16
ρ_{cal} (g/cm^3)	2.400	2.236	1.843
μ (mm^{-1})	11.973	10.800	8.169
F(000)	1584	824	3680
Reflections collected	4581	13647	77754
Independent reflections	2622 [R_{int} = 0.0296]	2638 [R_{int} = 0.0262]	15161 [R_{int} = 0.1262]
R_1 [$I > 2\sigma(I)$]	0.0183 [a]	0.0167 [a]	0.0450 [a]
wR_2 (all)	0.0455 [b]	0.0351 [b]	0.1053 [b]
GOF	1.083	1.170	0.986

[a] $R_1 = \Sigma| |F_o| - |F_c| |/ \Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2]/ \Sigma w(F_o^2)^2]^{1/2}$

	2[Pt^{II}(ppy)Sar]·CH_2Cl_2 (Crystal-G)	[Pt^{II}(ppy)Sar]·CH_2Cl_2 (Crystal-Y)
formula	$C_{29}H_{30}Cl_2N_4O_4Pt_2$	$C_{15}H_{16}Cl_2N_2O_2Pt$
formula weight	959.65	522.29
temperature (K)	200	200
crystal system	Monoclinic	Monoclinic
space group	*P*2(1)/c	*C*2/c
a / Å	9.8806(7)	23.7936(19)
b / Å	14.9744(11)	13.7569(11)
c / Å	21.8714(16)	10.2752(8)
α / º	90.00	90.00
β / º	102.4630(10)	93.9160(10)
γ / º	90.00	90.00
V / $Å^3$	3159.8(4)	3355.5(5)
Flack parameter	–	–
Z	4	8
ρ_{cal} (g/cm^3)	2.017	2.068
μ (mm^{-1})	9.053	8.688
F(000)	1816	1984
Reflections collected	35019	18081
Independent reflections	6970 [R_{int} = 0.0258]	3557 [R_{int} = 0.0223]
R_1 [$I > 2\sigma(I)$]	0.0198[a]	0.0175 [a]
wR_2 (all)	0.0457[b]	0.0429 [b]
GOF	0.996	1.036

[a] $R_1 = \Sigma| |F_o| - |F_c| |/ \Sigma|F_o|$. [b] $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2]/ \Sigma w(F_o^2)^2]^{1/2}$

Table S3. The hydrogen bond geometry (Å, deg) of 2[Pt^{II}(ppy)Sar]·CH_2Cl_2 (Crystal-G) and [Pt^{II}(ppy)Sar]·CH_2Cl_2(Crystal-Y).

Complex	***D*(–H)···*A***	***D*–H**	**H···*A***	***D*···*A***	***D*–H···*A***
2[Pt^{II}(ppy)Sar]·CH_2Cl_2 (Crystal-G)	N2–H1···O4^{i}	0.83(4)	2.16(4)	2.936(4)	155(4)
	N2–H1···O3^{i}	0.83(4)	2.58(4)	3.216(4)	134(4)
	N4–H15···O2	0.79(4)	2.27(4)	2.979(4)	150(4)
	N4–H15···O1	0.79(4)	2.45(4)	3.137(4)	145(4)
[Pt^{II}(ppy)Sar]·CH_2Cl_2 (Crystal-Y)	N2–H1···O1^{ii}	0.82(4)	2.64(4)	3.294(4)	138(3)
	N1–H1···O2^{ii}	0.82(4)	2.19(4)	2.963(4)	(4)158(4)

Symmetry codes: (i) x+1, y, z; (ii) x, -y+2, z-1/2.